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About the new method in theory of superconductivity I

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After discovery of isotope effect it became universally acceptable that the interaction of electrons with the lattice should play an essential role in the superconductivity phenomena.

Several interesting constructions (1, 2, 3) analyzing the system of electrons interacting with phonon field have been already made. In the present article we will show that by the method of path development proposed earlier for the theory of superfluidity it is possible to give a consistent theory of superconductive state. This partly confirms the results of work done by (3).

For simplicity of exposition we will proceed from the model proposed by H. Frölich (1) in which the Coulomb interaction obviously is disregarded and the dynamic system is characterized by Hamiltonian^{x)}.

$$H_{F2} = \sum_{k,s} E(k) a_{ks}^+ a_{ks} + \sum_q \omega(q) B_q^+ B_q + H_{int}$$

$$H_{int} = g \sum_{\substack{(k,s),s \\ (k',s) \\ k'-k=q}} \left(\frac{\omega(q)}{2V} \right)^{1/2} a_{ks}^+ a_{k's} B_q^+ + \text{comp},$$

where $E(k)$ - energy of an electron

$\omega(q)$ - energy of phonon

g - binding constant

V - volume

x) Here the system of units is such that $\hbar = 1$.

As is now very well known the usual theory of perturbation by the degree of binding constant is unacceptable, for the electron-phonon interaction, regardless of its smallness, appears to be quite essential near the Fermi surface. Therefore we will first of all perform some canonic transformation proceeding from the following considerations.

A remark should be made that the matrix elements corresponding to virtual production of "particles" from vacuum are always accompanied by energy denominators.

$$\left\{ E(k) + \dots + E(k_{2s}) + \omega(q_1) + \dots + \omega(q_2) \right\}^{-1}$$

in which $E(k) = [E(k) - E_F]$ presents

the energy of particle-electron $[E(k) > E_F]$ or of the hole $[E(k) < E_F]$ becoming small in Fermi surface. Such denominators usually are not "dangerous" and the integration by impulses $k_1, \dots, k_{2s}, q_1, \dots, q_r$ does not lead to divergence except the case where we have to deal with virtual process of production of one pair without phonons. Then, by the law of ~~conservation~~ ^{conservation} the particles of this pair will have oppositely directed impulses $\pm k$ and the energy denominator $[2E(k)]^{-1}$ becomes "dangerous" for integration. Their spins will also be oriented oppositely.

Therefore by choosing a canonic transformation one must be aware of the necessity to insure mutual compensation of graphs leading to virtual production from vacuum of a pair of particles with opposite impulses and spin orientations.

Now we will point out the analogy of situation we had in our theory of superfluidity when the nonideal Bose gas was examined. The same role then played the virtual production from the condensate of a pair of particles with

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$\pm K$ impulse. Then we used the linear transformation of Bose-amplitude, which was "mixing" b_q with b_{-q}^+ . Generalizing this transformation, let us introduce into presently examined case new Fermi amplitudes d :

$$d_{k0} = U_k a_{k, \frac{1}{2}} - V_k a_{-k, -\frac{1}{2}}^+$$

$$d_{k1} = U_k a_{-k, -\frac{1}{2}} + V_k a_{k, \frac{1}{2}}^+$$

or

$$a_{k, \frac{1}{2}} = U_k d_{k0} + V_k d_{k1}^+$$

$$a_{-k, -\frac{1}{2}} = U_k d_{k1} - V_k d_{k0}^+ \quad (I)$$

where U_k , V_k ~~are~~ real numbers related

$$\text{by } U_k^2 + V_k^2 = 1$$

It is easy to check, that such a transformation preserves all the Commutation properties of Fermi operators and therefore is canonic. We may say also that it presents a generalization of usual transformation. It helps to introduce new operators of production and ^{annihilation} cancellation of holes inside and of electrons outside the Fermi surface.

And really, suppose that

$$U_k = 1, \quad V_k = 0 \quad \text{for } E(k) > E_F$$

$$U_k = 0, \quad V_k = 1 \quad \text{for } E(k) < E_F$$

will result

$$d_{k0} = a_{k, \frac{1}{2}}, \quad d_{k1} = a_{-k, -\frac{1}{2}}, \quad E(k) > E_F$$

$$d_{k0} = -a_{-k, -\frac{1}{2}}^+, \quad d_{k1} = a_{k, \frac{1}{2}}^+, \quad E(k) < E_F$$

So that, for example d_{k0} outside the Fermi region (sphere) will be ^{an annihilation} cancellation operator for an electron with K impulse and k spin, and inside it will be ² cancellation

operator for a hole with $-K$ impulse and $-\frac{1}{2}$ spin. But in general case when $(u_k, v_k) \neq (0, 1)$ we are dealing with superposition of hole and electron.

Returning to the examination of Frolich's Hamiltonian, we notice that technically it will be more convenient for us not to ~~bind~~ ^{confine} ourselves with the relation:

$$\sum_{k,s} a_{ks}^+ a_{ks} = N_0$$

where N_0 is total number of electrons (and therefore we shall use an example which is typical for such a situation) i.e. we will introduce parameter λ having the role of chemical potential.

Then instead of H_0 we shall deal with Hamiltonian

$$H = H_0 - \lambda N \quad (2)$$

We shall define the parameter λ later in a manner that will give us in this condition

$$N = N_0 \quad (3)$$

After transforming H to new fermi - amplitudes we get:

$$H = U + H_0 + H_{int}$$

$$H_{int} = H_1 + H_2 + H_3$$

where U is a constant:

$$U = 2 \sum E(k) V_k^2 - 2 \lambda \sum V_k^2$$

and:

$$H_1 = \sum_{\substack{(k, k') \\ (k' - k = q)}} g \sqrt{\frac{\omega(q)}{2V}} \left\{ U_k V_k a_{k0}^+ a_{k'1}^+ + U_{-k} V_{-k'} a_{-k'0}^+ a_{-k1}^+ + \right. \\ \left. + U_{k'} V_k a_{k1} a_{k'0} + U_{k'} V_{-k} a_{-k'1} a_{-k0} \right\} B_q^+ + \text{Comp}$$

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$$H_2 = \sum_{\substack{(k, k') \\ (k' - k = q)}} g \sqrt{\frac{\omega(q)}{2V}} \left\{ U_k U_{k'} \alpha_{k_0}^+ \alpha_{k'_0} + U_k U_{-k'} \alpha_{-k_1}^+ \alpha_{-k'_1} \right. \\ \left. - V_k V_{k'} \alpha_{k_1}^+ \alpha_{k'_1} - V_k V_{-k'} \alpha_{-k_0}^+ \alpha_{-k'_0} \right\} B_q^+ + \text{comp.}$$

$$H_3 = \sum 2 [E(k) - \lambda] U_k V_k (\alpha_{k_0}^+ \alpha_{k_1}^+ + \alpha_{k_1}^+ \alpha_{k_0}^+)$$

$$H_0 = \sum [E(k) - \lambda] [U_k^2 - V_k^2] [\alpha_{k_0}^+ \alpha_{k_0} + \alpha_{k_1}^+ \alpha_{k_1}] + \sum \omega(q) B_q^+ B_q$$

Let us introduce occupation numbers

$$V_{k_0} = \alpha_{k_0}^+ \alpha_{k_0} \quad V_{k_1} = \alpha_{k_1}^+ \alpha_{k_1}$$

new quasi-particles, produced by α^+ operators. Then, "vacuum without interactions" i.e. the condition C_V in which:

$$H_0 C_V = 0$$

will obviously be the condition ~~the condition~~:

$$C_V = \prod_k \delta(V_{k_0}) \delta(V_{k_1})$$

with zero value for numbers V .

Also note that λ should be close to E_F , because $\lambda = E_F$ when interaction is absent, and that consequently the expression

$$\epsilon(k) = [E(k) - \lambda] [U_k^2 - V_k^2]$$

should become zero at the surface near the Fermi surface.

Now we can see that the virtual production process from vacuum of one pair of quasi-particle V_{k_0}, V_{k_1} without phonons will be "dangerous" in the meaning of previously given criteria for the corresponding energy denominator will be:

$$\frac{1}{2 \epsilon(k)}$$

To such a process directly leads the Hamiltonian H_3 which enclosing with vacuum gives graph ^{x)} of Fig. 1. The same process results also because of joint action H_1, H_2 . For example in the second order of binding constant g we have graphs shown in Fig. 2a.

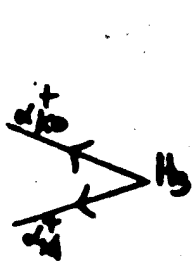


Fig. 1

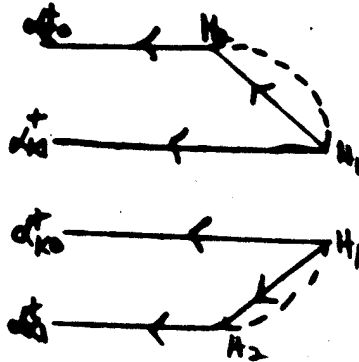


Fig. 2a

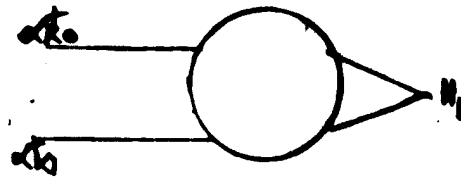


Fig. 2b

In higher orders graphs result of the type of Fig. 2b, where the circle designates bound part which cannot be divided into two bound parts connected only by two lines of one examined pair.

Using the previously deduced principle of compensation of dangerous graphs, we should set the sum of contributions from graphs of Fig. 1 and Fig. 2 equal to zero.

Hence we obtain an equation for determining U_k, V_k . Now we should not pay any attention to the graphs of Fig. 1 and 2 (and their conjugates) and therefore in developments of perturbation theory expressions with dangerous energy denominator will not appear. Now we shall develop an

x) Here we have used type of graphs examined in Hugenholtz's work

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equation for U_k, V_k of second order. In this approximation we have to compensate the graph of fig. 1 by graphs of fig. 2b. We will get:

$$2[E(k) - \lambda] U_k V_k + \mathcal{J}k = 0$$

where $\mathcal{J}k$ is the coefficient of $\alpha_{k_0}^+ \alpha_{k_1} C_V$ in the expression

$$-H_2 H_0^{-1} H_1 C_V$$

Rationalizing we find finally:

$$\{\tilde{E}(k) - \lambda\} U_k V_k = (U_k^2 - V_k^2) \frac{1}{2V} \sum_k g^2 \frac{\omega(k-k')}{\omega(k-k') + E(k) + E(k')} U_{k'} V_{k'}$$

where

$$\tilde{E}(k) = E(k) - \frac{1}{2V} \sum_k g^2 \frac{\omega(k-k')}{\omega(k-k') + E(k) + E(k')} (U_{k'}^2 - V_{k'}^2)$$

Remaining within acceptable approximation let us substitute in the denominator of right hand part

$$E(k) = \{E(k) - \lambda\} (U_k^2 - V_k^2)$$

by $\tilde{E}(k) = \{E(k) - \lambda\} (U_k^2 - V_k^2)$

Then, assuming

$$\tilde{E}(k) - \lambda = \xi(k)$$

let us write the resulting equation in the form

$$\xi(k) U_k V_k = (U_k^2 - V_k^2) \frac{1}{2(2\pi)^3} \int g^2 \frac{\omega(k-k')}{\omega(k-k') + E(k) + E(k')} U_{k'} V_{k'} d^3k' \quad (6)$$

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This equation obviously possesses a property of trivial solution

$$UV=0, (U, V) = (0, 1)$$

corresponding to "normal state". It does, nevertheless, give a solution of other type which becomes trivial when moving away from Fermi surface.

Designating

$$C(k) = \frac{1}{(2\pi)^3} \int d^3r \frac{\omega(k-k')}{\omega(k-k') + \tilde{\epsilon}(k) + \tilde{\epsilon}(k')} V_k U_{k'} d\vec{r}$$

we find from (6)

$$U_k^2 = \frac{1}{2} \left\{ 1 + \frac{\tilde{\epsilon}}{\sqrt{C(k)^2 + \tilde{\epsilon}^2}} \right\}, V_k^2 = \frac{1}{2} \left\{ 1 - \frac{\tilde{\epsilon}}{\sqrt{C(k)^2 + \tilde{\epsilon}^2}} \right\} \quad (7)$$

from where

$$U_k V_k = \frac{1}{2} \frac{C(k)}{\sqrt{C(k)^2 + \tilde{\epsilon}^2}}; \tilde{\epsilon} = \frac{\tilde{\epsilon}^2}{\sqrt{C(k)^2 + \tilde{\epsilon}^2}}$$

Therefore our equation leads to the next from:

$$C(k) = \frac{1}{2(2\pi)^3} \int d^3r \frac{\omega(k-k')}{\omega(k-k') + \tilde{\epsilon}(k) + \tilde{\epsilon}(k')} \cdot \frac{C(k')}{C(k) + \tilde{\epsilon}^2(k')} d\vec{r} \quad (8)$$

A remark should be made that this equation has its particular peculiarity when the solution of ψ approaches zero for

$$\exp \left\{ -\frac{A}{g^2} \right\}, \quad A = \text{const.} > 0$$

because the integral of right hand side of (8) becomes logarithmically divergent near the surface $\xi(k) = 0$ if assumed $C = 0$. In such a situation it is not difficult to obtain asymptotic form of solution for small g s:

$$C(k) = \tilde{\omega} e^{-\frac{k}{g}} \cdot \frac{1}{2} \int_0^1 \frac{\omega \{k_0 \sqrt{2(1-\theta)}\}}{\omega \{k_0 \sqrt{2(1-\theta)}\} + 1/300} d\theta \quad (9)$$

where $\rho = g^2 \frac{1}{\pi^2} \left(\frac{K^2}{2R} \right)_{K=K_0}, \quad E(K_0) = \lambda$

where

$$\ln \tilde{\omega} = \int_0^{\infty} \ln \left(\frac{1}{2\pi} \right) \frac{d}{d\xi} \left\{ \frac{1}{2} \int_0^1 \frac{\omega \{k_0 \sqrt{2(1-\theta)}\}}{\omega \{k_0 \sqrt{2(1-\theta)}\} + \frac{1}{3}} d\theta \right\} d\xi \quad (10)$$

Taking into account additional condition (3) and obtained (7), (9) for U, V it can be said, that

$$K_0 = K_F$$

Further, it is clear, that corrections for expression (5) stemming from substitution of appearing in it U_k, V_k for their "normal" significance:

$$U_k = \theta_g(k) = \begin{cases} 1, & |k| > K_F \\ 0, & |k| < K_F \end{cases}$$

$$V_k = \theta_F(k) = \begin{cases} 0, & |k| > K_F \\ 1, & |k| < K_F \end{cases}$$

(11)

will be exponentially small. Therefore in formulae (10) we can without loss of exactness substitute $\tilde{E}(k)$ by corresponding form for normal state and interpret the factor:

$$\frac{1}{2\pi} \left(\frac{k}{k_0} \right)_{k \rightarrow k_0} = \frac{1}{V} \left\{ \frac{V}{(2\pi)^3} \frac{4\pi k^2 dk}{dE} \right\}_0$$

as relative density $\frac{dn}{dE}$ number of electron level in infinitely narrow energy layer near Fermi surface.

Then:

$$\rho = g^2 \frac{dn}{dE} \quad (12)$$

Let us now proceed with calculation of ground state energy in second approximation. Of all the ~~terms~~ we must now account only for H_1 . We will get, consequently, for proper value of H in ground state

$$U = \langle G_V^\dagger H_1 H_0^{-1} H_1 G_V \rangle$$

$$= 2 \sum \{ E(k) - \epsilon \} V_k^2 \quad (13)$$

$$= \frac{1}{V} \sum_{k, k'} g^2 \frac{W(k-k) \{ V_k^2 V_{k'}^2 + V_k V_{k'} \}}{W(k-k) + \tilde{E}(k) + \tilde{E}(k')}$$

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Substituting the derived values for U_k , V_k , let us calculate the difference ΔE between the energies of ground state and normal state

We get:

$$\frac{\Delta E}{V} = - \frac{dN}{dE} \cdot \frac{\tilde{\omega}^2}{2} \exp\left(-\frac{2}{\beta}\right) \quad (14)$$

It is interesting to observe that this result coincides with Bardeen's results (3). It is only necessary to choose Bardeen's parameters u , V in a manner:

$$2\omega = \tilde{\omega} \quad , \quad V = g^2 \quad (15)$$

Let us construct now within acceptable approximations formula for energy of elementary excitation. We use for this excitation the ^{state} condition:

$$C_k = \alpha_{k0}^+ C_0$$

and subject it in usual manner ^{to} the theory of perturbation. We will get for the energy of elementary excitation with impulse K next expression

$$E_0(K) = E(K) - \langle G^+ H_{int} (H_0 - E(K))^{-1} H_{int} G \rangle_{bound}$$

rationalizing we get

$$E_0(K) = \tilde{E}(K) \left\{ 1 - \frac{g^2}{V} \sum_{K'} \omega(K-K') \frac{U_K^2 U_{K'}^2 + V_K^2 V_{K'}^2}{[\omega(K-K') + E(K')]^2 - E(K)} \right. \\ \left. + \frac{g^2}{V} 2 U_K V_K \sum_{K'} \frac{\omega(K-K') [\omega(K-K') + E(K')]}{[\omega(K-K') + E(K')]^2 - E(K)} U_{K'} V_{K'} \right\} \quad (16)$$

The first member, proportional to $\tilde{E}(k)$, does not have the same property and becomes zero at the Fermi surface. The second member at the Fermi surface is equal to

$$\int \frac{2\omega_k \sum_{\mathbf{k}} \frac{\mu(\mathbf{k}-\mathbf{k}')}{\omega(\mathbf{k}-\mathbf{k}') + \omega(\mathbf{k})}}{2\omega_k \omega(\mathbf{k})} \mu_k \mu_{k'} \\ = 2\omega_k \omega(\mathbf{k}) = C(k) = \tilde{\omega} e^{-\frac{1}{2}}$$

Hence, the energies of excited states are separated from the energy of ground state by a gap

$$\Delta = \tilde{\omega} e^{-\frac{1}{2}} \quad (17)$$

In Bardeen's work there are expressions of the type

$$2\tilde{\omega} e^{-\frac{1}{2}}$$

interpreted there as energy used for the destruction of "pair".

Let us examine now ground state with net current flow i.e. the condition of smallest energy among all possible conditions with a given impulse \vec{P} .

We need consequently to find proper value of H by additional condition:

$$\sum_{\mathbf{k}\mathbf{s}} \vec{k} a_{\mathbf{k}\mathbf{s}}^{\dagger} a_{\mathbf{k}\mathbf{s}} = \vec{P}$$

Instead of this, using the usual procedure, we introduce instead of scalar parameter λ another vector parameter \vec{U} , playing the role of average velocity and take the whole Hamiltonian in form:

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$$\begin{aligned}
 H &= H_{\text{int}} - \lambda \sum_{\vec{k}} a_{\vec{k}3}^+ a_{\vec{k}3} - \sum_{\vec{k}} (\vec{U} \cdot \vec{k}) a_{\vec{k}3}^+ a_{\vec{k}3} \\
 &= \sum_{\vec{k}} \{E(\vec{k}) - \vec{U} \cdot \vec{k} - \lambda\} a_{\vec{k}3}^+ a_{\vec{k}3} + \sum_{\vec{q}} \omega_{\vec{q}} b_{\vec{q}}^+ b_{\vec{q}} + H_{\text{int}}
 \end{aligned}
 \tag{18}$$

\vec{U} is defined from condition

$$\sum_{\vec{k}} \vec{k} a_{\vec{k}3}^+ a_{\vec{k}3} = \vec{P}$$

In so far as our discussion is concerned, we have to deal with only a small area of Fermi surface; hence, we can assume here for simplicity

$$E(\vec{k}) = \frac{k^2}{2m} + D, \quad D = E_F - \frac{k_F^2}{2m}$$

and then in final formulae to let

$$m = \left(\frac{k}{\frac{dE}{dk}} \right)_{k=k_F}$$

But then

$$E(\vec{k}) - (\vec{U} \cdot \vec{k}) = E(\vec{k} - m \vec{U}) - \frac{m \vec{U}^2}{2}$$

and therefore, if in the region of \vec{k} impulses we perform a translation

$$\vec{k} \rightarrow \vec{k} + \vec{U}m, \quad a_{\vec{k}3} \rightarrow a_{\vec{k}+m\vec{U}3}$$

(19)

and substitute

$$\lambda \rightarrow \lambda + \frac{m \vec{U}^2}{2}$$

then the Hamiltonian (13) will be in form of (2) and the vector \vec{U} drops out. We are getting to the case of ground state with zero impulse. Furthermore for the study of ground state with net current flow we need conduct no new investigation, but it will be sufficient in previously obtained formulae to do reverse conversion of (19).

Hence we are convinced, for example, that the energy of ground state with net current flow with average velocity \vec{U} differs from the energy of ground state without net current flow by amount $N \frac{m U^2}{2}$. Excitations are separated from energy of ground state with net current flow by a gap

$$\Delta_v = \Delta - K_F U > \Delta - K_F / |\vec{U}|$$

Consequently, if

$$K_F / |\vec{U}| < \Delta$$

the ground state with net current flow, even though it possesses energy greater than the ground state without net current flow (we do not account yet ^{for} the action of magnetic field) nevertheless it appears stable in relation to excitations.

Therefore we are convinced that in the model being examined there is a property of superconductivity.

Few more remarks. In our method of investigation we should have assumed parameter ρ to be small in order to be able to limit ourselves to asymptotic approximations.

As was shown by V. V. Tolmachev and S. V. Pablikoff (5) through a method not using the assumption of ρ being small; when $\rho > \frac{1}{2}$ the velocity of sound becomes imaginary i.e. lattice becomes unstable. In cases, when the lattice is so rigid that electron-phonon interaction does not show any appreciable effects on the phonon energy, the parameter must be small. Even when $\rho = \frac{1}{2}$ the quantity $e^{\gamma/\rho}$ is equal to 1/55. This, in our opinion, explains the smallness of the magnitude of energy gap and therefore also of critical temperature.

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Furthermore, when the Fröhlich's Hamiltonian is supplemented in obvious manner by a term of Coulomb interaction then it becomes necessary summing up of electron-hole graphs of the Helman-Brückner type in order to secure the appearance of shielding.

For preliminary estimate we could introduce Coulomb interaction into Hamiltonian immediately in shielded form and treat it also by means of perturbation theory. We would get then actually the same formulae we obtained previously; but it would be necessary to change in them g^2 for

$$g^2 \rightarrow \frac{1}{2} \int_0^1 V_e(k, \sqrt{2(1-\epsilon)}) d\epsilon$$

where $V_e(k)$ Fourier - form of shielding function.

Hence, we can be immediately convinced that Coulomb interaction counteracts the appearance of superconductivity.

In conclusion I feel it is my pleasant duty to express my gratitude to: I. N. Subarev, V. V. Tolmachev, S. V. Tiablikoff, U. A. Cerkovnikoff for valuable criticism and suggestions.

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